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LOW TEMPERATURE DIAMAGNETISM OF ELECTRONS IN A CYLINDER

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Prepared in January 1953

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Abstract

The exact eigenfunctions are found for an electron in a cylindrical container in the presence of a uniform axial magnetic field. The eigenvalue spectrum, while superficially similar to that in free space, is so essentially different that the statistical properties of an electron assembly in the cylinder are entirely different from those derived in previous work. It is therefore of interest to use an integration approximation in computing the energy of the assembly at 0°K. It turns out to have a very strong size-dependent paramagnetic term, and the reasons for this are carefully explained. The work lends support to the view that the observed diamagnetism of electrons in the superconducting state cannot be understood in terms of any free electron approximation, and that interactions with the lattice potential play an essential role.

Introduction

Previous work on the quantum mechanical properties of electrons in a magnetic field has been characterized by a wide variety of conflicting results. In two important papers recently (1) Osborne and Steele have shown how carefully one has to handle the statistics in order to avoid some of these conflicts. However their work, and apparently much previous work, has treated the boundary value problem of fitting the eigenfunctions to the walls of the container in an approximate fashion: Osborne in particular used the WKB method, and in common with all previous discussions, the concept of localized reflected electron orbits is basic to the work.

The present paper stems from the idea that this concept of reflected localized orbits is inapplicable to the low temperatures pertaining in superconductivity work. The "fuzziness" of the Fermi surface in wave-number space, representing the possible uncertainty in the momentum of any particular electron, is too sharp to provide localized wave-groups in ordinary space for the conducting electrons: the uncertainty in position is necessarily at least of the order 10^{-5} cm. Especially for small cylinders it would therefore be quite unsafe to picture an electron as a particle capable of being reflected in a definite orbit, and the WKB approximation could hardly be regarded as reliable.

There is very good reason to believe that the errors caused by using

approximate eigenfunctions and their unrealistic energy spectra may
cause errors at least as serious as those attacked by Osborne and
Steele in developing the statistics of the problem. It therefore
seemed worth while to seek the exact eigenfunctions in a closed cyl-
inder with an axial magnetic field, using no approximations at all, so
that the concept of localized orbits need never enter the argument.
These exact eigenfunctions have been found in the form of modified
Bessel functions whose nodes can be made to fit the walls of the cyl-
inder by the proper choice of energy, thereby quantizing the latter.
The resulting eigenvalue spectrum is superficially similar with that
usually assumed ($\underline{2}$), but differs significantly. The difference is
such that the Fermi statistics of the assembly of electrons in the
cylinder cannot be even approximately similar with that assumed in
previous work.

Because of this it has seemed worth while at the present time to
find the energy of an assembly at $0^{o}K$ using standard integration approx-
imations, and to leave to future work the more exact development using
the method of Osborne. It would in fact be of interest to use the integ-
ration approximation to find the energy as a function of temperature, but
even the calculations at $0^{o}K$ are extremely tedious and we have decided to
forego the further work for the time being.

The exact eigenfunctions for a cylinder

Assuming the spin to be separable, we write the Hamiltonian operator without spin (3):

$$\mathcal{H} = -(\hbar^2/2M)\nabla^2 - i\hbar(eH/2Mc)\partial/\partial\phi + \tfrac{1}{2}r^2(eH/2Mc)^2 \qquad (1)$$

where M is the mass and $-e$ the charge of the electron, H is the magnetic field directed along the z-axis. We seek solutions of the Schrödinger equation in the form

$$\psi = R(r)\, e^{ikz}\, e^{im\phi} \qquad (2)$$

where m is an integer, positive or negative, and k is the wave-number corresponding to plane waves propagated along the z-axis of the cylinder. The equation for $R(r)$ reduces to

$$R'' + R'/r + (K^2 - m^2/r^2 - \alpha^2 r^2)R = 0 \qquad (3)$$

where $\qquad \alpha = eH/2\hbar c$

$$(4)$$

and $\qquad K^2 = 2ME/\hbar^2 - k^2 - 2m\alpha$

E being the total energy.

In the limit of zero magnetic field eq.(3) is the Bessel equation; we shall express the solutions in a form that displays their relation with the Bessel functions as clearly as possible. To do this it is convenient to introduce the following change of variable:

$$x = Kr, \quad X(x) = R(r), \quad \beta = \alpha/K^2 \qquad (5)$$

The equation for R then becomes the following equation for X:

$$X'' + X'/x + (1 - m^2/x^2 - \beta^2 x^2)X = 0 \qquad (6)$$

This equation is soluble by series integration, the result being

$$X(x) = e^{-\frac{1}{2}\beta x^2} J_m^*(x) \tag{7}$$

where

$$J_m^*(x) = \sum_{n=0} (-1)^n B_{mn} (\tfrac{1}{2}x)^{|m|+2n} / n!(n+|m|)! \tag{8}$$

with $$B_{mn} = \prod_{j=0}^{n-1} \left\{ 1 - 2\beta(1+|m|+2j) \right\} \tag{9}$$

Clearly when $\beta = 0$ the factors B_{mn} become unity and the function $J_m^*(x)$ reduces to the Bessel function of order m. Reverting to the original variables the unnormalized eigenfunctions are

$$\psi = e^{ikz} e^{im\phi} e^{-\frac{1}{2}\alpha r^2} J_m^*(Kr) \tag{10}$$

These are the only solutions that are well-behaved both at the origin and as the radius of the cylinder is increased indefinitely. They are exact.

It is obvious that at small enough magnetic fields the perturbed Bessel functions $J_m^*(Kr)$ have zeroes not far removed from the zeroes of the Bessel functions $J_m(Kr)$. As the value of β is increased by increasing the magnetic field it is of course possible for the spectrum of zeroes not only to move considerably, but also to break up into a completely different spectrum. In the present paper we confine ourselves to the simplest case where the field is small enough to be regarded as only a small perturbation in the sense that the spectrum of zeroes of J_m^* is essentially similar with that of the zeroes of the Bessel functions. We prove also that actual experimental fields are small in this sense.

On the above understanding we can fit the wave functions into a closed cylinder of radius a by requiring that K have one of the values given by the zeroes of the perturbed Bessel functions:

$$K = K_{mj}, \quad \text{where} \quad J_m^*(aK_{mj}) = 0 \tag{11}$$

Through eq.(4) this in turn determines the possible energies of the electron in the closed cylinder:

$$E_{kmj} = \hbar^2 k^2/2M + \hbar^2 K_{mj}^2/2M + m e\hbar H/Mc \tag{12}$$

These eigenvalues can be determined as exactly as we wish to compute the zeroes of the perturbed Bessel functions.

To the first order in β the coefficients B_{mn} in eq.(9) are

$$B_{mn} = 1 - 2\beta n(n+|m|) + \ldots \tag{13}$$

and it is easy to prove from this that

$$J_m^* = J_m(1 + \tfrac{1}{2}\beta x^2) \tag{14}$$

Therefore for small fields the zeroes of J^* are identical with those of the Bessel functions J, and the effect of small fields on the eigenvalues is completely taken care of by the last term in eq.(12), the quantities K_{mj} being independent of the field.

We may note numerically that K is of the order 10^7 before it makes any appreciable contribution to the energy, while α is of the order 10^7 times H. Thus β will remain less than 10^{-2} for all fields less than 10^5 gauss, and the above conclusions should be valid for all fields yet employed experimentally.

The eigenvalue spectrum (12) is essentially different from that appropriate to free space, which is (3)

$$E_{kn} = \hbar^2 k^2/2M + (n+\tfrac{1}{2})e\hbar H/Mc \tag{15}$$

In this spectrum n is an unlimited positive integer arising from oscillator terms. In our spectrum for the cylinder there is a new term arising from the zeroes of the Bessel functions, and m is an angular momentum quantum number that may have either positive or negative values. At $0^\circ K$ the n of eq.(15) is limited by the Fermi energy ζ_0:

$$\zeta_0 = (n_0+\tfrac{1}{2})e\hbar H/Mc \tag{16}$$

but the m of eq.(12) is restricted by the boundary in a quite different fashion, as follows.

For large values of $|m|$ the first two zeroes of the Bessel functions and therefore also of the perturbed Bessel functions $J_m^*(x)$ occur at the arguments

$$x_{1m} = K_{1m} a = |m| + 1.856|m|^{1/3} + \ldots$$
$$x_{2m} = K_{2m} a = |m| + 3.245|m|^{1/3} + \ldots \tag{17}$$

In order to fit the first zero of J_m^* to the cylinder one therefore needs a larger value of K_{1m} the larger $|m|$, and so the maximum energy sets a limit on the maximum $|m|$ even for zero magnetic field. By contrast eq.(16) leaves n_0 unlimited when the magnetic field vanishes. From (12) and (17) the maximum $|m|$ is m_0 where, in absence of magnetic field

$$\zeta_0 = (m_0 + 1.856 \, m_0^{1/3})^2 \, \hbar^2/2Ma^2 \tag{18}$$

At this point one can already predict that there will be anomalous size effects in the present problem because of the cube root term in m_0.

One can also see qualitatively from eq.(17) how the boundary causes
the presence of so-called reflected orbits. It is clear that for large
values of $|m|$ the spacing between the zeroes becomes progressively small
compared with the radius a as $|m|$ increases. For large $|m|$ values the
peak of the function $J_m^*(aK_{1m})$ becomes very narrow and confined to radii
very close to a. This is true for both positive and negative m-values.
Of course there is no orbit on the present picture; every eigenfunction
is actually reflected at the cylinder because it has to have a node
there. For this reason we may also expect a much higher paramagnetic
term than that given by the orbit concept.

The Fermi Assembly

We now wish to construct the Fermi region in quantum number space,
within which all states are occupied at $0^\circ K$ if we have an assembly of N
electrons in the cylinder.   The Fermi surface is given by eq.(12) in
the form

$$(\hbar^2/2M)\left\{ K_{jm}^2 + (\pi n/L)^2 \right\} + 2m\rho = \zeta \qquad (19)$$

where ζ is the Fermi energy, and we have written

$$\rho = e\hbar H/2Mc \qquad (20)$$

and $k = \pi n/L$. L being the length of the cylinder, n and j are
integers.   Consider now all states of given m obtained by varying j,
i.e. the number of nodes of J_m^* inside the cylinder.   For large values

of j the nodes occur as follows:

$$aK_{jm} = \pi(j + 3/4) \qquad m \text{ even}$$
$$aK_{jm} = \pi(j + 1/4) \qquad m \text{ odd} \tag{21}$$

and are asymptotically independent of m. Since only a relatively small number of states occur at small values of j, and we are going to use an integration approximation, we may use eq.(21) in the approximate form

$$aK_{jm} = \pi j \tag{22}$$

and double the number of states compared with the number of integers j. To this approximation eq.(19) becomes

$$(\hbar^2/2M)\left\{(\pi j/a)^2 + (\pi n/L)^2\right\} + 2m\rho = \zeta \tag{23}$$

Comparing (21) with (17) we note next that for a given positive m, the values of j must suffer a cut-off below j_o where

$$j_o = m + 1.856 \, m^{1/3} \tag{24}$$

For smaller values of j than this the first zero of J_m^o falls beyond r = a. For negative values of m we have exactly the same situation with the minimum value of j given by

$$j_o = -m + 1.856(-m)^{1/3} \tag{25}$$

These last two equations represent two cylinders intersecting along the n-axis in number space, and the Fermi region is that portion of the number space lying between these two cylinders and cut off by the Fermi surface eq.(23). This is illustrated in Figure 1.

The number of states is eight times the volume of the Fermi region above the n-m plane: a factor of two for the two m-values per j-value in

$(\hbar^2/2M)\left\{(\pi j/a)^2 + (\pi n/L)^2\right\} + 2m\varrho = \xi$

$\pi j_0 = -m + 1.856(-m)^{1/3}$

$\pi j_0 = -m + 1.856\, m^{1/3}$

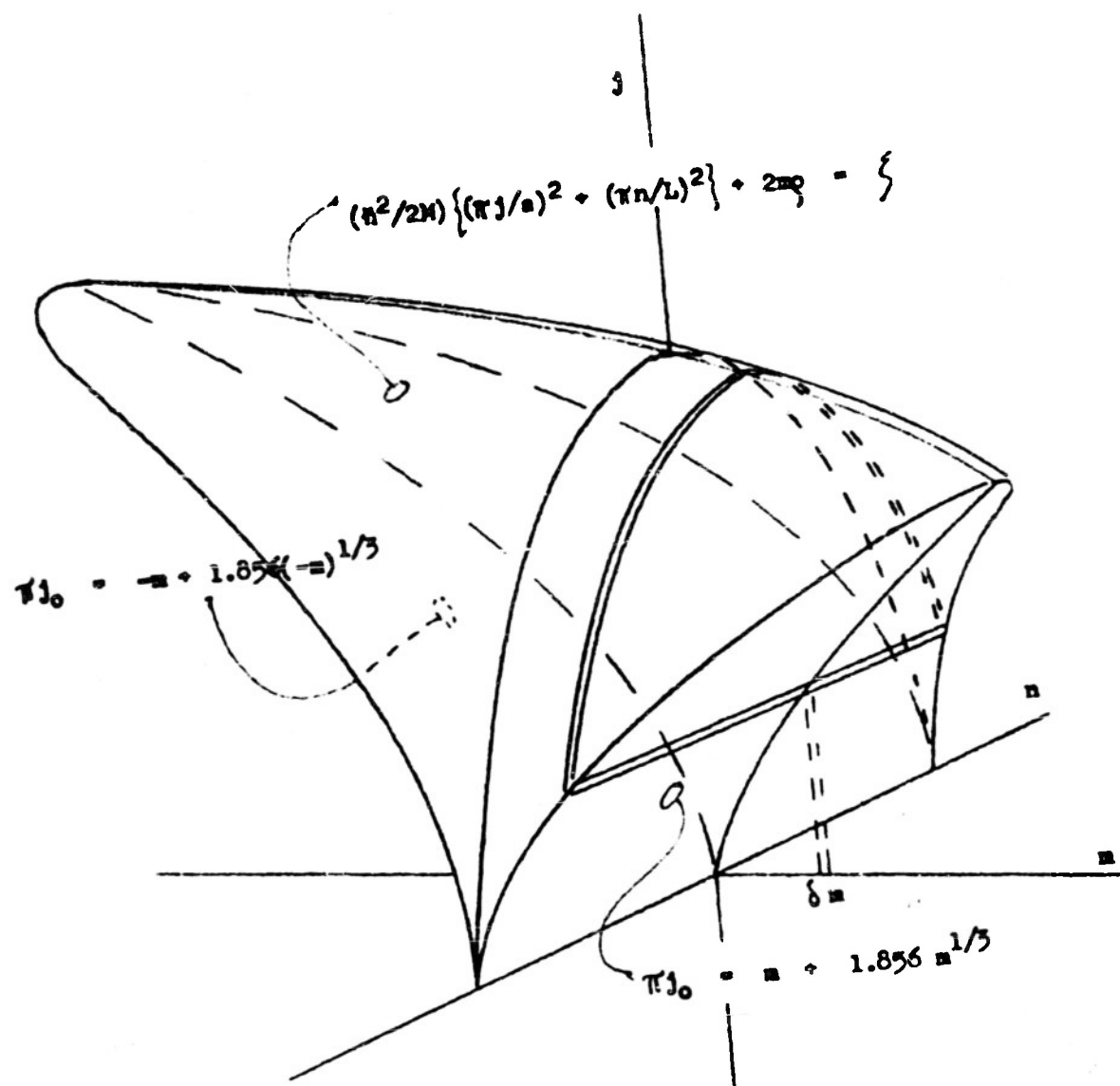FIGURE 1

eq.(21), a factor of two for the spin, and a factor of two to include the negative j-values.

Our first objective is to find the volume of the Fermi region and so determine the Fermi energy in terms of the total number N of electrons. We find the volume for positive m-values first, the volume for negative m-values is then obtained simply by reversing the sign of ρ, and the total volume is the sum of these. It therefore contains no term linear in ρ, and in every approximation we must count all terms quadratic in ρ to be able eventually to find the susceptibility of the assembly.

Write $\qquad x = \hbar k/\sqrt{2M} = \hbar m\pi/L\sqrt{2M}, \qquad y = \hbar j\pi/a\sqrt{2M}$ $\qquad$ (26)

and the equation of the Fermi surface

$$x^2 + y^2 + 2m\rho = \zeta \qquad (27)$$

The total number of states in the Fermi region is

$$N = v \iiint dx\, dy\, dm \qquad (28)$$

where $\qquad v = 16MaL/\pi^2\hbar^2$.

Take parabolic sections parallel to the x-y plane - see Figure 1. The number of states on the positive side of that plane is then

$$N_o = 2v \iint (\zeta - 2m\rho - y^2)^{\frac{1}{2}}\, dy\, dm \qquad (29)$$

where the range of integration over y is

$$(m + 1.856\, m^{1/3})/g \leq y \leq (\zeta - 2m\rho)^{\frac{1}{2}} \qquad (30)$$

with $\qquad g = a\sqrt{2M}/\hbar$

Write $\qquad z = (m + 1.856\, m^{1/3})/g \qquad (31)$

and m_o for the solution of

$$m_o + 1.856\, m_o^{1/3} = g(\zeta - 2m_o\rho)^{\frac{1}{2}} \qquad (32)$$

then K_4 can be written as the sum of the following three integrals:

$$K_{41} = \int_0^{m_0} \pi \bar{n}(\xi - 2m\rho)dm = \pi(\tfrac{2}{3}m_0 - \tfrac{1}{2}\Gamma\rho m_0^2) \tag{33}$$

$$K_{42} = -\pi \int_0^{m_0} m(\xi - 2m\rho - m^2)^{\tfrac{1}{2}} dm \tag{34}$$

$$K_{43} = -\pi \int_0^{m_0} (\xi - 2m\rho) \arcsin\{m(\xi - 2m\rho)^{-\tfrac{1}{2}}\} dm \tag{35}$$

To evaluate K_{42} and K_{43} it is convenient to use x as the variable instead of m, or the ratio

$$t = x/x_0 \tag{36}$$

where

$$x_0 = (\xi - 2m_0\rho)^{\tfrac{1}{2}} \tag{37}$$

Remembering that only large values of m are important, we can write in place of eq.(31)

$$m = gx - 1.856 (gx)^{1/3} \tag{38}$$

Moreover we can expand the square root in the integrand of eq.(34) as follows:

$$(\xi - 2m\rho - x^2)^{\tfrac{1}{2}} = x_0(1 - t^2)^{\tfrac{1}{2}} + g\rho(1 - t)/(1 - t^2)^{\tfrac{1}{2}}$$
$$- 1.856\, g^{1/3}\rho x_0^{-2/3}(1 - t^{1/3})(1 - t^2)^{-\tfrac{1}{2}}$$
$$- (1/8)\rho^2 g^2 x_0^{-1}(1 - t)^2(1 - t^2)^{-3/2} \tag{39}$$

Combining (39) and (38) we can express (34) in the form of a sum of eight integrals all of which are well-behaved and either elementary or reducible to elliptic integrals that can be readily evaluated*.

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* See the Appendix

The result is

$$N_{+2}/w \; = \; 0.011 g/z_0$$
$$+ \; \rho\left\{ -0.125(gz_0)^2 + 0.388(gz_0)^{4/3} - 0.197(gz_0)^{2/3} \right\}$$
$$+ \; (\rho/z_0)^2\left\{ 0.0177(gz_0)^3 - 0.033(gz_0)^{7/3} \right\} \tag{40}$$

To evaluate N_{+3} we expand the integrand, using

$$\xi \; - \; 2m\rho \; = \; z_0^2 \; + \; 2\rho(m_0 - m)$$

and the following development of the arcsin:

$$\mathrm{arcsin}\left\{ z(\xi - 2m\rho)^{-\frac{1}{2}} \right\} \; = \; \mathrm{arcsin}\, t \; - \; (\rho/z_0^2)(m_0 - m)(1 - t^2)^{-\frac{1}{2}}$$
$$+ \; (3/2)(\rho/z_0^2)^2(m_0 - m)^2(1 - t^2)^{-\frac{1}{2}}$$
$$+ \; \tfrac{1}{2}t(\rho/z_0^2)^2(m_0 - m)^2(1 - t^2)^{-3/2} \; + \; \ldots \tag{41}$$

We then express the whole integrand in terms of t by writing

$$m_0 - m \; = \; gz_0(1 - t) \; - \; 1.856(gz_0)^{1/3}(1 - t^{1/3}) \tag{42}$$

Neglecting only terms involving ρ^3 or higher orders, these steps result in twenty four integrals which are again elementary or can be reduced to elliptic integrals. We find

$$N_{+3}/w \; = \; - \, 0.5708 gz_0^3 \; + \; 0.521(gz_0)^{1/3}z_0^2$$
$$+ \; \rho\left\{ 0.2146(gz_0)^2 - 1.2755(gz_0)^{4/3} + 1.541(gz_0)^{2/3} \right\}$$
$$+ \; (\rho/z_0)^2\left\{ 0.1073(gz_0)^3 + 1.188(gz_0)^{7/3} + 1.610(gz_0)^{5/3} \right\} \tag{43}$$

To express N_{+1} in terms of the Fermi energy we need the solution of eq.(32) for m_0:

$$m_0 \; = \; g\xi^{\frac{1}{2}} \; - \; 1.856(g\xi^{\frac{1}{2}})^{1/3}$$
$$- \; (\rho/\xi)\,(g\xi^{\frac{1}{2}})^2 \; - \; 1.238(g\xi^{\frac{1}{2}})^{4/3} \; + \; \tfrac{1}{2}(\rho/\xi)^2(g\xi^{\frac{1}{2}})^3 \; \ldots \tag{44}$$

To express the other parts of N_+ in terms of ξ we need the expansion for z_0 derived from eq.(44) and eq.(37):

$$z_0/\xi^{\frac{1}{2}} = 1 - (\rho/\xi)\left\{g\xi^{\frac{1}{2}} - 1.856(g\xi^{\frac{1}{2}})^{1/3}\right\}$$
$$+ (\rho/\xi^{\frac{1}{2}})^2\left\{\frac{1}{2}(g\xi^{\frac{1}{2}})^2 + 0.619(g\xi^{\frac{1}{2}})^{4/3}\right\} \ldots \qquad (45)$$

Carrying out these developments we then add the three parts of N_+, double the terms of even order in ρ and remove the terms linear in ρ, the result is the total number in the whole Fermi region:

$$N/w\xi = 2.02(g\xi^{\frac{1}{2}}) - 4.82(g\xi^{\frac{1}{2}})^{1/3} +$$
$$(\rho/\xi)^2\left\{13.14(g\xi^{\frac{1}{2}})^3 + 8.00(g\xi^{\frac{1}{2}})^{7/3} - 11.84(g\xi^{\frac{1}{2}})^{5/3} + 2.34(g\xi^{\frac{1}{2}})\right\} \quad (46)$$

Writing in the definitions of g and w from eqs.(30) and (28), and solving eq.(46) for the Fermi energy ξ we find:

$$\xi = 1.540(N/V)^{2/3}\hbar^2/2M + 2.11(N/V)^{4/9}(\hbar^2/2M)a^{-2/3}$$
$$- \rho^2(2M/\hbar^2)\left\{0.434a^2 + 2.265(N/V)^{-2/9}a^{4/3} - 2.91(N/V)^{-4/9}a^{2/3}\right\} \quad (47)$$

where $V = \pi a^2 L$ the volume of the cylinder.

The Energy of the Fermi Assembly

The energy of an assembly of N electrons filling the Fermi region on the positive side of the x-y plane is

$$E_+ = w \iiint(x^2 + y^2 + 2m\rho)dx\,dy\,dm \qquad (48)$$

The energy on the negative side is obtained from this be reversing the sign of ρ in the final expression. The total energy therefore has no term linear in ρ, and again all developments must be carried far enough to include all terms quadratic in ρ. Taking the same elements of volume

as for the N-integrations we have the three contributions to E_+:

$$E_{+1} = (2/3)\pi \iint (\xi - 2m\rho - y^2)^{3/2} \, dy \, dm \tag{49}$$

$$E_{+2} = 2\pi \iint y^2 (\xi - 2m\rho - y^2)^{\frac{1}{2}} \, dy \, dm \tag{50}$$

$$E_{+3} = 4w\rho \iint m (\xi - 2m\rho - y^2)^{\frac{1}{2}} \, dy \, dm \tag{51}$$

The range of integration over y is the same as in eq.(29). The first of these contributions integrates immediately over y to yield the four

integrals $E_{+1} = \sum_j E_{1j}, \qquad j = 1, 2, 3, 4.$ 9(52)

$$E_{11} = (\pi/8)w \int_0^{m_0} (\xi - 2m\rho)^2 \, dm$$
$$= w\xi^2 m_0 \pi/8 - w\rho \xi m_0^2 \pi/4 + w\rho^2 m_0^2 \pi/6 \tag{53}$$

$$E_{12} = (w/6) \int_0^{m_0} z(\xi - 2m\rho - z^2)^{3/2} \, dm \tag{54}$$

$$E_{13} = -(w/4) \int_0^{m_0} z(\xi - 2m\rho)(\xi - 2m\rho - z^2)^{\frac{1}{2}} \, dm \tag{55}$$

$$E_{14} = -(w/4) \int_0^{m_0} (\xi - 2m\rho)^2 \arcsin\left\{ z(\xi - 2m\rho)^{-\frac{1}{2}} \right\} \, dm \tag{56}$$

Using eq.(38) and the same kind of expansion as eq.(39), the integral in eq.(54) breaks up into ten elementary integrals that can be evaluated without difficulty. The similar expansions for the integrand of eq.(55) yields twenty more integrals, and the expansions for eq.(56) yield thirty integrals to obtain E_{+1}.

   The second contribution E_{+2} of eq.(50) integrates over y to yield the sum of the following four contributions:

$$E_{21} = E_{11}, \quad E_{22} = 3E_{12}, \quad E_{23} = E_{13}, \text{ and } E_{24} = E_{14} \tag{57}$$

The final contribution E_{*3} of eq.(51) integrates over y to yield three contributions E_{3j}, $j = 1,2,3$. Of these E_{31} integrates directly over m, E_{32} involves an expansion and develops into eleven elementary integrals, and E_{33} develops similarly into seventeen integrals. Totalling all these contributions to the energy, doubling the terms even in ρ and removing those linear in ρ, we derive the energy E of the Fermi assembly:

$$E/w\xi^2 = 0.324(g\xi^{\frac{1}{2}}) - 2.67(g\xi^2)^{1/3} +$$
$$(\rho/\xi)^2 \left\{ -9.08\Lambda(g\xi^{\frac{1}{2}})^3 + 7.84(g\xi^{\frac{1}{2}})^{7/3} + 31.44(g\xi^{\frac{1}{2}})^{5/3} \right\} \qquad (58)$$

In the derivation of this result of course the expansion (45) has to be used before the terms linear in ρ are removed.

If we take only the leading terms in (58) and (46) we find for the mean energy per electron at absolute zero in first approximation of zero magnetic field and large volume:

$$E/N = 0.462\xi \qquad (59)$$

We now use eq.(47) for the Fermi energy, and the definitions (30) and (28) for g and w, and eq.(19) for ρ in eq.(58)   and obtain the final expression for the energy of the assembly at 0^oK:

$$E/N = 0.354(N/V)^{2/3}(\hbar^2/2M) + 0.36(N/V)^{4/9}(\hbar^2/2M)a^{-4/3} -$$
$$(2a^2H^2/Mc^2)\left\{ 2.49a^2 - 1.98(N/V)^{-2/9}a^{4/3} - 10.5(N/V)^{-4/9}a^{2/3} \right\} \qquad (60)$$

The approximations upon which the various power-series developments are based depend for their validity on the magnetic terms being found

small compared with the leading term. Numerically it turns out that
this requires, in eq.(60), that a^2H^2 be not much larger than 0.01.
If therefore we were interested in cylinders of radius no larger than
10^{-3} cm. the magnetic field could be as high as 100 gauss; the result
is therefore of interest in a general discussion of superconductivity
which exists only for small magnetic fields.

Discussion

The susceptibility resulting from eq.(60) is clearly paramagnetic
and for macroscopic specimens extremely large compared with the orbital
diamagnetism in free space. The comparison is strongly size dependent.
From eq.(60) we have the susceptibility, neglecting the smaller terms:

$$X_{cyl} = 9.96\ e^2\ a^2\ (N/V)/Mc^2 \tag{61}$$

and in free space (3)

$$X_{free} = -0.105 e^2 (N/V)^{1/3}/Mc^2 \tag{62}$$

Even for cylinders as small as 10^{-5} cm in radius the quantity (61) is
roughly ten thousand times the magnitude of X_{free}.

One can understand this surprising result in the following way.
In the first splace, as mentioned earlier, the classical picture of
localized orbits is inapplicable. On that picture, and on the picture
quantum picture using the WKB approximation, the reflected orbits either
exactly or very nearly balance the unreflected orbits, so that the net
susceptibility is very small. On the present picture using the exact
eigenfunctions in the cylinder, every state is reflected by the boundary
because it has to have a node there. The division into reflected and

unreflected orbits can not now be made. When one carefully checks which
integrals actually lead to the paramagnetic term it turns out that eq.(32)
is directly to blame. The major contribution comes immediately from the
quadratic term in (ρ/ξ) in eq.(44), the solution of eq.(32). This
equation arises directly from the relation between the circular and the
radial nodes of the Bessel functions and is inherent in the exact solut-
ion of the problem. By contrast the solution for free space involves no
such cut-off in the Fermi region. The Fermi region obtained from the
spectrum of eq.(15) is cut off only at $n = 0$ and the maximum of n
occurs at the vertex of the parabola $y^2 + 2n\rho = \xi$: $n_o = \xi/2\rho$.

The contrast between this and eq.(44) should lead us to expect
entirely different results in the cylinder. Incidentally the factor g
appearing in eq.(32) and (44) is immediately responsible for the size-
dependence of the paramagnetic term.

One could reverse the sign of this term and so obtain a very large
diamagnetism for example by changing the square root in eq.(32) into
some rational power greater than unity. This would follow for a model
relationship replacing eq.(16) having a leading term of the form

$$x_{1m} = m^{1/\nu}$$

with $\nu > 2$. Any potential field capable of producing such a radical
alteration in the zeroes of the Bessel functions could hardly be handled
by simple first order perturbation theory starting from the wave functions
obtained here for the field free cylinder.

The smaller terms depending on H in eq.(60) are diamagnetic. They arise from the cube root terms in eq.(32), and are many orders smaller than eq.(61). These diamagnetic terms can formally become comparable with the paramagnetic term only by setting the radius of the cylinder less than 10^{-6} or 10^{-7} cm; but the power developments used in approximating the various integrals would no longer be valid. The assembly of 1000 electrons considered by Basden and quoted in Osborne's paper ($\underline{1}$) was found to be diamagnetic, and this would agree with the present formal result.

The second non-magnetic term in eq.(60) is not without interest. It also arises from the cube root term in the behaviour of the nodes. While it is many orders smaller than the leading term except at very small radii, it is such as to stablise the whole assembly against break-up into separate smaller sub-assemblies. It may serve to justify our taking the entire population of the cylinder in one single Fermi assembly and applying the exclusion principle to all the electrons. Without such a term one could equally well assume that the population breaks up into domains within which the exclusion principle operates, but between which electrons in different domains disregard eachother. This latter is possible when using periodic boundary conditions in a rectangular enclosure, the boundary being then nothing more than a convenient fiction.

One conclusion seems very definite. It is quite impossible for free electrons in a cylinder to exhibit the type of diamagnetism that we need

to understand superconductivity. This diamagnetism certainly exists experimentally in the limit of small fields under the conditions of validity of the formula (60). It seems certain therefore that this diamagnetism must be a result of the interaction between the electrons and the lattice potential, and not a property describable approximately in terms of the electrons alone. The lattice potential must in fact alter drastically the relationship between the circular and radial nodes of the eigenfunctions and so completely change the shape of the Fermi region in wave-number space - which of course it obviously does - and diamagnetism must be the result of this.

It would be of further interest to study our present problem for very strong fields. This could be done by developing the various integrands in powers of (ξ/ρ) instead of (ρ/ξ). The corresponding terms in E/N depending on magnetic field would form a polynomial in negative powers of H, and could conceivably have a large number of zeroes, so yielding the de Haas van Alphen effect. The exact way of handling this however would be by the method of Osborne; it would be extremely complicated owing to the awkward shape of the Fermi region, and the present writer does not plan to make the attempt.

References

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     M.O. Steele   Physical Review 88   p.451   November 1   1952

2.   J.H.Van Vleck   The Theory of Electric and Magnetic Susceptibilities
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3.   F. Seitz   The Modern Theory of Solids
                         Mc Grew Hill   New York 1940

Caption to Figure 1.

The Fermi Region in Wave Number Space

j   -   index for circular nodes
m   -   index for radial nodes
k   -   index for plane nodes

Appendix

Most of the integrals encountered in this work can be reduced to the following form:

$$K(n) = \int_0^1 x^{n/3} \arcsin X \, dX$$

Below we tabulate the needed numerical values. Some of these had to be obtained by direct summation of series expansions of the integrand; the others were found by reduction to elliptical integrals.

TABLE

n	K(n)
- 5	3.114
- 4	1.606
- 2	0.840
- 1	0.6765
0	0.5708
1	0.491
2	0.431
3	0.3927
4	0.360
5	0.330
6	0.3014
7	0.272
10	0.218